Consistent picture for resonance-neutron-peak and angle-resolved photoemission spectra in high-T_c superconductors

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The spectra observed in angle-resolved photoemission spectroscopy measurements are examined together with the resonance peak observed in neutron scattering, based on the slave-boson approach to the t-t'-J model. We show that the peak/dip/hump features arise from the scattering of electrons by collective spin excitations which, at the same time, give rise to the neutron resonance mode. The doping dependences and the dispersions of the peak/dip/hump positions are shown to be consistent with experiments. The recently observed $\cos(6\theta)$ deviation from the pure d wave is also discussed based on the renormalization by spin fluctuations.

Both angle-resolved photoemission spectroscopy (ARPES) and neutron scattering experiments have played important roles in the studies of high-T_c superconductors. It has been shown by ARPES that the spectral line shape possesses a peak/dip/hump structure in the superconducting (SC) state.[1,2] The anomalous momentum, temperature, and doping dependences of the spectral line shape suggest that electrons are strongly coupled to collective excitations centered at (π,π) and these collective excitations are related to the pairing interaction.[3] On the other hand, the most prominent feature of the spin susceptibility observed in neutron scattering studies is the sharp resonance peak at (π,π) in the superconducting or pseudogap states.[4–6] It has been speculated,[3,7] from a comparison of these two kinds of experimental data, that the collective excitations are the resonance modes in the neutron scattering experiments. This idea has been further explored qualitatively in a phenomenological spin-fermion model,[8] in which the resonance mode is identified as the propagating collective spin excitations and the scattering of electrons by these spin modes gives rise to the anomalous spectral line shape. It has also been examined based on the fluctuation-exchange (FLEX) approximation for the one-band Hubbard model.[9] Using the slave-boson theory for the t-t'-J model, Brinckmann and Lee[10] have investigated the spin resonance and its evolution with doping.

A recent ARPES study reveals the specular dependences of the peak, dip, and hump energies with doping.[11] Furthermore, a small $\cos(6\theta)$ (θ is the Fermi surface angle) deviation from the pure d-wave structure is observed.[12] These results and their correlation with the mode energy inferred from neutron data are the essential ingredient for a consistent picture of the ARPES line shape and the neutron data. In this paper, we examine these issues and show that they can be quantitatively reproduced based on the slave-boson approach to the two-dimensional (2D) t-t'-J model.

The model reads

$$H=-\sum_{\langle ij\rangle,\sigma} tc^{\dagger}_{i\sigma}c_{j\sigma}-\text{H.c.}-\sum_{\langle ij\rangle',\sigma} t'c^{\dagger}_{i\sigma}c_{j\sigma}$$
$$-\text{H.c.}+J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{1}$$

where $\langle ij\rangle$ denotes the nearest-neighbor (NN) bond and $\langle ij\rangle'$ the next-NN bond. In the slave-boson method, the physical electron operators $c_{i\sigma}$ are expressed by slave bosons b_i carrying the charge and fermions $f_{i\sigma}$ representing the spin; $c_{i\sigma}=b^{\dagger}_i f_{i\sigma}$. We consider the d-wave SC state with the order parameters $\Delta_{ij}=\langle f_{i\uparrow}f_{j\downarrow}-f_{i\downarrow}f_{j\downarrow}\rangle$ and $\chi_{ij}=\Sigma_\sigma\langle f^{\dagger}_{i\sigma}f_{j\sigma}\rangle$, in which bosons condense: $b_i\rightarrow\langle b_i\rangle=\sqrt{\delta}$ (δ is the hole concentration).[14] Then, the mean-field Hamiltonian of Eq. (1) is

$$H_m=\sum_{k\sigma}\epsilon_k f^{\dagger}_{k\sigma}f_{k\sigma}-\sum_k\Delta_k(f^{\dagger}_{k\uparrow}f^{\dagger}_{-k\downarrow}+\text{c.c.})$$
$$+2NJ'(\chi_0^2+\Delta_0^2), \tag{2}$$

where the dispersion for fermions,

$$\epsilon_k=-2(\delta t+J'\chi_0)[\cos(k_x)+\cos(k_y)]$$
$$-4\delta t'\cos(k_x)\cos(k_y)-\mu,$$

and the gap $\Delta(k)=2J'\Delta_0[\cos(k_x)-\cos(k_y)]$, with $J'=3J/8$. The mean-field parameters χ_0, Δ_0 and the chemical potential μ for different doping δ are obtained from a self-consistent calculation.[14]

In the above mean-field calculation, we have set $\langle\mathbf{S}_i\rangle=0$.[14] In order to consider the response to external magnetic and electric fields, we include the antiferromagnetic (AF) fluctuation by writing $H=H_m+H'$, where $H'=H-H_m$, and treating H' as a perturbation to H_m. In the Hartree-Fock approximation, this reproduces the mean-field

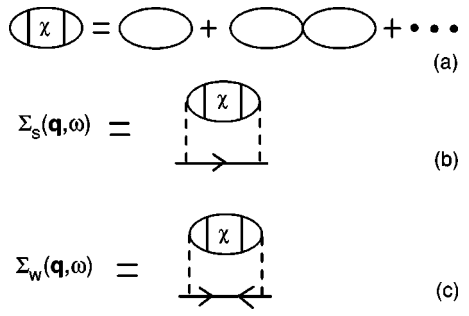

FIG. 1. Feynman diagrams for (a) the RPA to the spin susceptibility coming from particle-hole excitations and (b) and (c) the lowest-order contribution to the self-energy from fermion-spin excitation scatterings.

results.[15] Here, we consider the scattering of electrons off spin fluctuations in H'. As a first step, we calculate the spin susceptibility in the random-phase approximation (RPA) as shown in Fig. 1(a),

$$\chi(\mathbf{q},\omega)=\chi_0(\mathbf{q},\omega)/[1+\alpha J(\mathbf{q})\chi_0(\mathbf{q},\omega)]. \tag{3}$$

Here $J(\mathbf{q})=J(\cos q_x+\cos q_y)$ and $\chi_0(\mathbf{q},\omega)$ is the unperturbed spin susceptibility which is calculated from the fermionic bubbles representing particle-hole excitations. Following Ref. 10, we choose $\alpha=0.34$ in order to set the AF instability at $\delta=0.02$, which is the experimentally observed value. The fermionic self-energy is obtained from the lowest-order contribution of the scatterings of fermions off spin fluctuations. In the SC state, there are two different self-energies Σ_s and Σ_w as shown in Figs. 1(b) and 1(c), which renormalize the fermionic dispersion and the SC gap, respectively. In the previous study,[8] only Σ_s is included in their calculations. We will show that the inclusion of Σ_w will lead the otherwise flat doping dependence of the ARPES peak to be consistent with experiments. The fermionic Green's function is calculated by $G_f(\mathbf{k},i\omega)=[G_{f0}^{-1}(\mathbf{k},i\omega)+(\Delta_k+\Sigma_w)^2G_{f0}(-\mathbf{k},-i\omega)]^{-1}$ with $G_{f0}(\mathbf{k},i\omega)=[i\omega-\epsilon_k-\Sigma_s(\mathbf{k},i\omega)]^{-1}$. In the SC state, bosons condense and the physical electron Green's function can be approximated by $G(\mathbf{k},\omega)\approx\delta G_f(\mathbf{q},\omega)$. Then, the spectral function of electrons is calculated from the retarded Green's function as $A(\mathbf{k},\omega)=-(1/\pi)\mathrm{Im}\,G(\mathbf{k},\omega)$. Numerical calculations are performed at low temperature $T=0.005J$, with $t=2J, t'=-0.45t$, and $J=0.13$ eV.

We first analyze the imaginary part of the spin susceptibilities at $\mathbf{Q}=(\pi,\pi)$. It develops sharp resonance peaks for various doping densities. This result has been reported in Ref. 10. In the framework of the *d*-wave BCS theory, the origin of these peaks has been discussed.[10,16,17] Essentially, the peak arises from a collective spin excitation mode corresponding to $1+\alpha J(\mathbf{Q})\mathrm{Re}\ \chi_0(\mathbf{Q},\omega)=0$ and negligibly small $\mathrm{Im}\,\chi_0(\mathbf{Q},\omega)$. It is due to a steplike rise of $\mathrm{Im}\,\chi_0$ at its gap edge and then a logarithmic singularity in $\mathrm{Re}\,\chi_0$ via the Kramers-Kronig relation. This singularity shifts downward the collective mode energy and leads it to situate in the spin gap, so no damping is expected for the mode. The steplike rise in $\mathrm{Im}\,\chi_0$ arises from the flat band (extended van Hove singularity) which is observed near $(\pi,0)$ (Ref. 18) and the property that $\Delta_{\mathbf{k}+\mathbf{Q}}=-\Delta_{\mathbf{k}}$ for transition momentum $\mathbf{Q}$ due to the *d*-wave gap symmetry.[17]

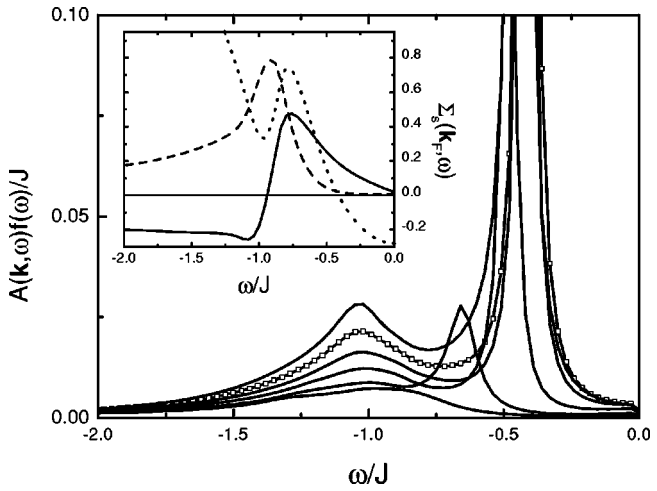

FIG. 2. Photoemission spectra $A(\mathbf{k},\omega)f(\omega)$ at $k=(\pi,0),(\pi,0.15\pi),(\pi,0.225\pi),(\pi,0.3\pi),(\pi,0.4\pi),(\pi,0.5\pi)$ (from the up to down lines). The inset shows the frequency dependence of the fermion self-energy Σ_s at $k_F=(\pi,0.15\pi)$ (Fermi wave vector). The solid line corresponds to its real part and the dashed line to its imaginary part. Also shown in the inset is $P(k_F,\omega)$ (see text) which is denoted by the dotted line.

The line shape $A(\mathbf{q},\omega)f(\omega)$ [$f(\omega)$ is the Fermi distribution function] of electrons coming from the scatterings by spin fluctuations for doping $\delta=0.12$ are shown in Fig. 2. The results are plotted for several wave vectors $k=(\pi,0),(\pi,0.15\pi),\ldots,$ down to $(\pi,0.5\pi)$. Clear peak/dip/hump structures are present at and near $(\pi,0)$. In order to understand the origin of the peak/dip/hump structure, we plot the self-energy Σ_s (Σ_w is qualitatively similar to Σ_s) at the Fermi wave vector k_F for doping $\delta=0.12$ in the inset of Fig. 2. The solid line denotes its real part Σ_s', while the dashed line its imaginary part Σ_s''. The corresponding line shape at k_F is expressed by the line with open squares in the main panel. Due to the coupling to the spin resonance mode, the whole structure of the self-energy Σ_s is very similar to that of the unperturbed spin susceptibility χ_0 (for a comparison, see Fig. 2 in Ref. 17). When frequency $|\omega|$ is below about $0.5J$, Σ_s'' is equal to zero. Above $0.5J$, a steplike rise can be seen and is followed by a decrease. Consequently, Σ_s' has a peak at about the center of the steplike rise of Σ_s''. The quasiparticle energy is given by the pole of the Green's function, which is the solution ω of the equation $P(k_F,\omega)=\mathrm{Re}\{[\omega-\Sigma_s(k_F,\omega)]^2-[\Delta_{k_F}+\Sigma_w(k_F,\omega)]^2\}=0$. We also show $P(k_F,\omega)$ (dotted line) in the inset of Fig. 2. The lowest-binding-energy solution of the pole equation $P(k_F,\omega)=0$ is $\omega=-0.42J$. Meanwhile, the damping of this mode which is proportional to Σ_s'' and Σ_w'' approaches zero. Therefore, it gives rise to a quasiparticle mode which is denoted by the sharp low-binding-energy peak in the line shape shown in Fig. 2. As $|\omega|$ increases further, the pole equation does not satisfy anymore. Near the end of the steplike rise in Σ_s'', $P(k_F,\omega)$ reaches its local maximum; meanwhile the imaginary part of the self-energy is also near its maximum, and therefore a dip appears. It indicates that the dip is caused by the steplike rise in the imaginary part of the self-energy. After the dip, $P(k_F,\omega)$ decreases with $|\omega|$, and near $\omega=-1.0J$, it reaches a local minimum. This leads to the broad higher-binding-energy hump.

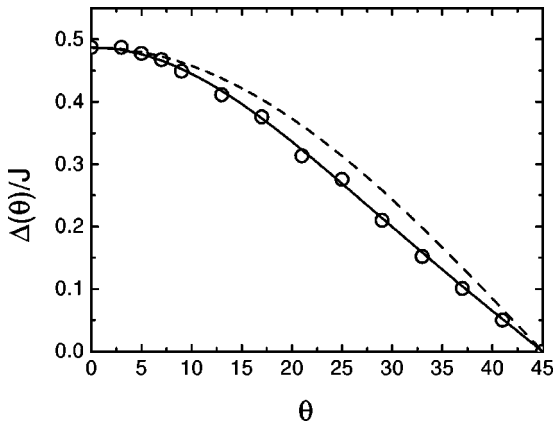

FIG. 3. The renormalized gap size vs the Fermi surface angle θ for $\delta=0.08$. The open circles are our results. The solid line is the fit using the gap function $\Delta(\theta)=\Delta_{\max}[B\cos(2\theta)+(1-B)\cos(6\theta)]$ with $B=0.94$ and the dashed line with $B=1.0$.

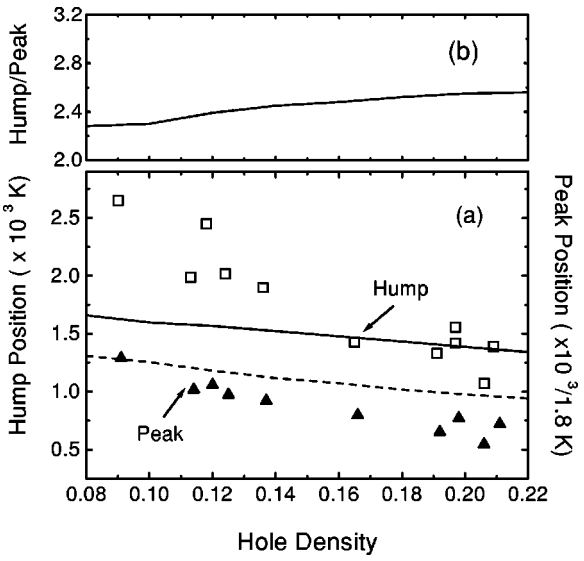

FIG. 4. Doping dependences of the energy scales for the hump and the peak at $(\pi,0)$. (a) Doping dependences of the hump and peak positions. The open squares and the solid triangles are experimental data for the hump and peak positions from Ref. 11, respectively. (b) Doping dependence of the ratio of the hump position to the peak position.

We now discuss the dispersion of the hump/dip/peak structure. At the momentum range below and slightly above the Fermi wave vector $(\pi,0.15\pi)$, the low-binding-energy peak nearly does not disperse with k. Above $(\pi,0.3\pi)$, the peak starts to move to higher binding energy but cannot move further than the dip seen around k_F. Then, it disappears gradually with the further increasing of k, due to the unavailable quasiparticle states above the Fermi surface at low temperatures. As a result, the dip also disappears gradually. These behaviors were observed in experiments.[11] The position of the peak determines the normalized gap size due to spin fluctuations. In Fig. 3, we show a typical dependence of the renormalized gap magnitude on the Fermi surface angle θ, which is the angle between k_F and k_x. In general, the next-order deviation from the d wave starts from $\cos(6\theta)$ and can be described by the form $\Delta(\theta)=\Delta_{\max}[B\cos(2\theta)+(1-B)\cos(6\theta)]$. The numerical values of B obtained in our approach are around 0.88–0.94, which agree roughly with the range of B found in Ref. 12. However, a more detailed analysis shows that the doping dependence of B has the opposite trend as that reported in Ref. 12. This discrepancy shows up in the doping dependence of $\Delta(\theta)$ near the node. While our $\Delta(\theta)$ is determined by the minimum gap locus via measuring the peak position, what is measured in experiments is usually the leading-edge gap. It is known that the width of the peak increases as one approaches $\theta=\pi/4$.[13] The leading-edge gap thus may incorporate the change of the width. The width determined from our approach appears to be much less broad in comparison to what is found in Ref. 12. Especially the measured peaks around $\pi/4$ reported in Ref. 12 seem to be overwhelmingly broad such that only the leading edges appear to change with doping (see Fig. 1 in Ref. 12). This may explain the failure of the RPA in the explanation of the doping dependence of B.

In Fig. 4(a), we show the doping dependence of the positions of the hump and the peak, and compare our results with the experiment.[11] One can see that our result for the peak is in reasonably good agreement with the experiment. We note that, if we just include the self-energy Σ_s in our calculation as was done in Ref. 8, a doping *independence* for the peak positions is obtained. Hence the renormalization of the gap by including Σ_w is important. The magnitude of the position of the hump and its trend with the doping variation are also consistent with the experiment, although the slope of the curve of hump versus hole density is flatter than the experimental result. The dependence of the ratio between the hump and peak energy at $(\pi,0)$ on doping concentrations is shown in Fig. 4(b). A flat variation for a wide doping level is seen. This result again agrees with the experiment.[11] In the above calculations, the adjustable parameters are α, which is fixed by the experimental observation on the AF instability, and the experimental energy resolution, which is stimulated to be $\Gamma=0.02J$. Other parameters are chosen according to well-known values. We find that the structure of the ARPES spectra and the peak and hump positions are not subject to the change of Γ, when it is below $0.07J$. So these results are quite satisfactory.

An important quantity addressed in the ARPES experiments is the peak-dip separation, which is shown to be close to the mode energy of the neutron peak.[11] Unlike the peak and hump positions, however, the dip position is sensitive to Γ. When Γ increases, the position of the local minimum in $P(k_F,\omega)$ increases and the quasiparticle peak broadens. As a result, the dip position and consequently the peak-dip separation increase. On the other hand, the position of the neutron scattering peak does not change for different Γ; it just becomes broad. So this comparison is also sensitive to Γ. In Fig. 5, we show the comparison of the peak-dip separations for $\Gamma=0.02J$ and $0.06J$, with the mode energy calculated in spin susceptibility. They have a similar dependence on the doping density. Furthermore, the peak-dip separation approaches the resonance mode energy when Γ increases. In the case of $\Gamma=0.06J$, both have a close magnitude in a wide doping range. As noted above, the dip stems from the steplike edge in Σ_s'' which is in turn caused by the coupling to the collective spin mode. On the other hand, this spin resonance mode also arises from the steplike edge in $\mathrm{Im}\,\chi_0$ which is

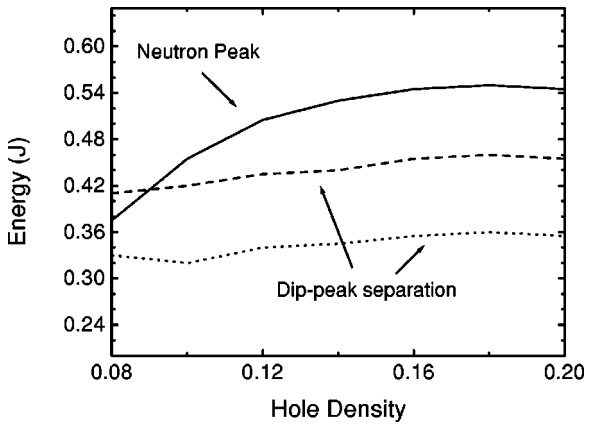

FIG. 5. Comparison between the doping dependences of the dip-peak separation in the ARPES spectra at $(\pi,0)$ and the neutron resonance mode energy. The dashed line is the result for $\Gamma = 0.06J$ and the dotted line for $\Gamma = 0.02J$.

due to the extended van Hove singularity near $(\pi,0)$ and the *d*-wave symmetry. Therefore, an intimate relation between them is suggested. Thus, our result seems to provide a consistent picture for the spin resonance peak and the hump/dip/peak structure based on the spin excitations in a *d*-wave superconductor.

Recently, White *et al.*[19] have investigated the effect of nonmagnetic Zn impurities on the line shape of $Bi_2Sr_2Ca(Cu_{1-x}Zn_x)O_{8+\delta}$ by ARPES experiment. They found that the dip is diminished with Zn doping. According to previous studies by one of the authors (Li),[17] Zn doping will wash out the van Hove singularity and cause the decays of quasiparticle states. So the enhancement in $\mathrm{Re}\,\chi_0$ and the steplike rise in $\mathrm{Im}\,\chi_0$ will be suppressed. As a result, no clear resonance neutron peak appears at certain Zn doping concentration.[17] Because the dip is suggested to come from the coupling to the spin resonance mode here, the disappearance of the dip upon Zn doping may be naturally explained in the present framework.

It is quite encouraging that our results fits several kinds of ARPES and neutron scattering data with correct trend and reasonable magnitude. Therefore, our investigation represents a natural extension to the work of Brinckmann and Lee,[10] which addressed the doping dependence of the resonance peak in neutron scattering. Our approach is different from the phenomenological study by Abanov and Chubukov.[8] It is based on the one-loop correction to the t-t'-J mean-field theory. Meanwhile, the result presented here further furnishes a quantitative basis in comparison to their qualitative study. We also note that the slave-boson mean-field theory of the 2D t-t'-J model and a one-loop calculation by just including the residual AF fluctuations produce qualitativly similar results to that obtained by the self-consistent FLEX scheme on the 2D Hubbard model.[9] Since the t-J model is identical to the large-U Hubbard model, this may suggest that the slave-boson approach to the t-t'-J model captures some essential physics related to high-T_c cuprates.

In summary, based on the slave-boson approach to the t-t'-J model, we show that the anomalous peak/dip/hump structure observed in the ARPES experiments arises from the coupling of quasiparticles to collective spin excitations, which gives rise to the resonance peak in neutron scattering experiments. Our investigation seems to give a consistent explanation for the resonance neutron peak and the ARPES spectra based on the spin excitations in a *d*-wave superconductor.

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